Control Design Analysis of Tubular Chemical Reactors

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The paper presents some results concerning analysis of steady-state and dynamic behaviour of tubular chemical reactors. The main aim of the proposed procedure is to choose an acceptable controlled output for a given control input with regard to controller design purposes.

Tubular chemical reactors are units frequently used in chemical and biochemical industry. From the system engineering point of view tubular chemical reactors belong to a class of nonlinear distributed parameter systems and their mathematical models are described by nonlinear partial differential equations. The simplification, modelling and simulation of such plants were presented by many authors, *e.g. Friedly* [1], *Luyben* [2], and *Ingham et al.* [3]. Some relationships between modelling and control of these systems can be found in works of *Stephanopoulos* [4] and *Seborg* [5].

It is well known that the control design of tubular reactors is a considerable complex. The control problems are due to the nonlinearity, the distributed nature of the description, and high sensitivity of the steady-state profiles to the input changes. In addition, the dynamic characteristics may exhibit a changing sign of the gain in various operating points, the time delay as well as non-minimum phase behaviour. Some control methods for the systems with mentioned input-output properties were proposed (*e.g.* Robust Control and Predictive Control), however, they are often undesirable for some control reasons.

Consider a system with one control input and many outputs, the task of the analysis is to find a suitably controlled output variable having good properties with respect to a control application. For this reason the following conditions can be required:

– constant sign of the gain for varying operating point during control,

– minimum phase input-output behaviour,

– the shortest time delay among all outputs.

Basic properties of the reactor depend on the reaction taking place inside. Therefore, a previous analysis is necessary for every assumed reaction type. Here, an exothermic reaction A → B → C is considered with the component B as a product and C as an undesired one.

This paper presents the simulation results of steady-state and dynamic analysis of the tubular chemical reactor important for control analysis and design.

MODEL OF THE PLANT

Consider an ideal plug-flow tubular chemical reactor with a simple exothermic consecutive reaction A → B → C in the liquid phase and with countercurrent cooling. Heat losses and heat conduction along the metal wall of tubes are assumed to be negligible, but dynamics of the metal wall of tubes are significant. All densities, heat capacities, and heat transfer coefficients are assumed to be constant. Under above assumptions, the reactor model can be described by five partial differential equations of the form

$$\frac{\partial c_A}{\partial t} + v_r \frac{\partial c_A}{\partial z} = -k_1 c_A \tag{1}$$

$$\frac{\partial c_B}{\partial t} + v_r \frac{\partial c_B}{\partial z} = k_1 c_A - k_2 c_B \tag{2}$$

$$\frac{\partial T_r}{\partial t} + v_r \frac{\partial T_r}{\partial z} = \frac{q_r}{(\rho c_p)_r} - \frac{4U_1}{d_1 (\rho c_p)_r}(T_r - T_w) \tag{3}$$

$$\frac{\partial T_w}{\partial t} = \frac{4}{(d_2^2 - d_1^2)(\rho c_p)_w}[d_1 U_1(T_r - T_w) + d_2 U_2(T_c - T_w)] \tag{4}$$

$$\frac{\partial T_c}{\partial t} - v_c \frac{\partial T_c}{\partial z} = \frac{4m d_2 U_2}{(d_3^2 - m d_2^2)(\rho c_p)_c}(T_w - T_c) \tag{5}$$

Table 1. Parameter Values and Steady-State Input Values

$d_1 = 0.02$ m	$d_2 = 0.024$ m	$d_3 = 1$ m
$m = 1200$	$L = 8$ m	$v_r = 0.398$ m s^{-1}
$\rho_r = 985$ kg m^{-3}	$\rho_w = 7800$ kg m^{-3}	$\rho_c = 998$ kg m^{-3}
$c_{pr} = 4.05$ kJ kg^{-1} K^{-1}	$c_{pw} = 0.71$ kJ kg^{-1} K^{-1}	$c_{pc} = 4.18$ kJ kg^{-1} K^{-1}
$U_1 = 2.8$ kJ m^{-2} K^{-1} s^{-1}		$U_2 = 2.56$ kJ m^{-2} K^{-1} s^{-1}
$k_{10} = 5.61 \times 10^{16}$ s^{-1}	$E_1/\boldsymbol{R} = 13477$ K	$h_1 = 5.8 \times 10^4$ J mol^{-1}
$k_{20} = 1.128 \times 10^{18}$ s^{-1}	$E_2/\boldsymbol{R} = 15290$ K	$h_2 = 1.8 \times 10^4$ J mol^{-1}
$c_{A0}^s = 2.85$ kmol m^{-3}	$T_{r0}^s = 323$ K	$T_{c0}^s = 293$ K

with initial conditions

$$c_A(z,0) = c_A^s(z), \ c_B(z,0) = c_B^s(z),$$
$$T_r(z,0) = T_r^s(z), \ T_w(z,0) = T_w^s(z), \ T_c(z,0) = T_c^s(z)$$

and boundary conditions

$$c_A(0,t) = c_{A0}(t), \ c_B(0,t) = c_{B0}(t) = 0,$$
$$T_r(0,t) = T_{r0}(t), \ T_c(L,t) = T_{cL}(t)$$

Here t is the time, z is the axial space variable, c are concentrations, T are temperatures, v are fluid velocities, d are diameters, ρ are densities, c_p are specific heat capacities, U are heat transfer coefficients, m is the number of tubes, and L is the length of the reactor. The subscripts are $(\cdot)_r$ for the reactant mixture, $(\cdot)_w$ for the metal wall of tubes, $(\cdot)_c$ for the coolant, and the superscript is $(\cdot)^s$ for steady-state values.

The reaction rates and the heat of reactions are expressed as

$$k_j = k_{jo} \exp\left(\frac{-E_j}{\boldsymbol{R}T_r}\right), \quad j = 1, 2 \qquad (6)$$

$$q_r = h_1 k_1 c_A + h_2 k_2 c_B \qquad (7)$$

where k_0 are pre-exponential factors, E are activation energies, h are reaction enthalpies, and $\boldsymbol{R}$ is the gas constant.

The coolant volumetric flow rate q_c, which will be taken as the control input, is contained in the term $v_c = q_c/A_c$. Here A_c is a free cross-sectional area of the reactor shell.

The mean temperature can be expressed as

$$T_m(t) = \frac{1}{L} \int_0^L T_r(z,t) \mathrm{d}z \qquad (8)$$

Practically, the temperatures T_r may be measured only at some given points z_i. Then the mean temperature will be computed from the equation

$$T_m(t) = \frac{1}{n_1} \sum_{i=1}^{n_1} T_r(z_i, t) \qquad (9)$$

All parameters and steady-state input values at the basic operating point, which were used for simulations, are shown in Table 1.
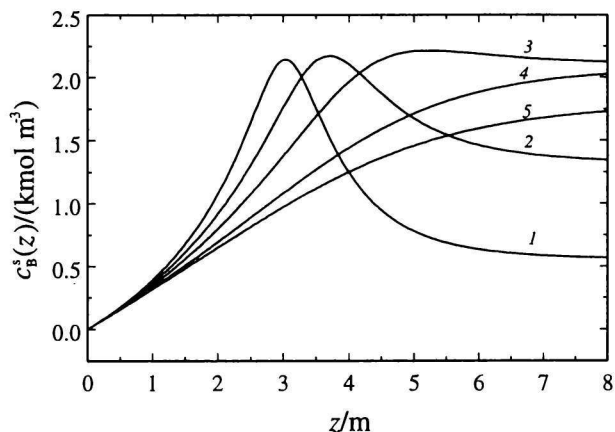

Fig. 1. Product concentration profiles for various coolant flow rates in a steady state. $q_c^s/(\text{m}^3 \text{ s}^{-1}) = 0.225$ (*1*), 0.25 (*2*), 0.275 (*3*), 0.3 (*4*), 0.325 (*5*).

SIMULATION RESULTS

Steady-State Analysis Results

The reactor steady-state characteristics were obtained by solution of eqns (*1—9*) under conditions $\partial(\cdot)/\partial t = 0$. Remaining differential terms were replaced by their limit-differenced equivalents. The initial conditions were computed by a standard iterative optimization procedure.

The influence of the coolant flow rate upon both, the product concentration and temperature profiles is illustrated in Figs. 1 and 2, respectively. The product concentration profiles for various values of the inlet temperature are shown in Fig. 3. All above results demonstrate sensitivity of all profiles in a steady state to changes of the inputs.

The curve of the dependence of the product outlet concentration upon the temperature shown in Fig. 4 gives the maximum for the certain mean temperature. It means that there exists an optimum mean temperature which enables to obtain the maximum product outlet concentration. This fact is significant in connection with a possible process control strategy.

Dynamic Analysis Results

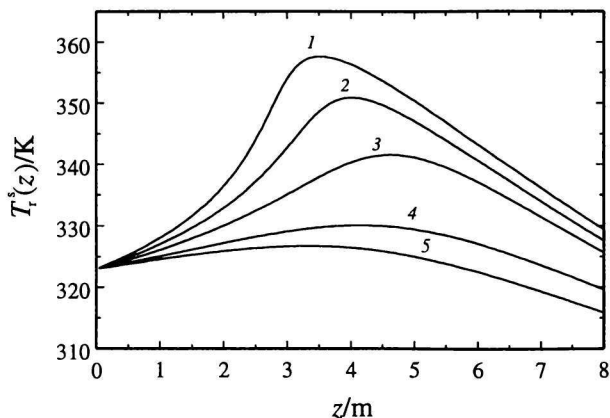For dynamic analysis purposes only one input and

Fig. 2. Temperature profiles for various coolant flow rates in a steady state. $q_c^s/(m^3\ s^{-1}) = 0.225\ (1),\ 0.25\ (2),\ 0.275\ (3),\ 0.3\ (4),\ 0.325\ (5)$.
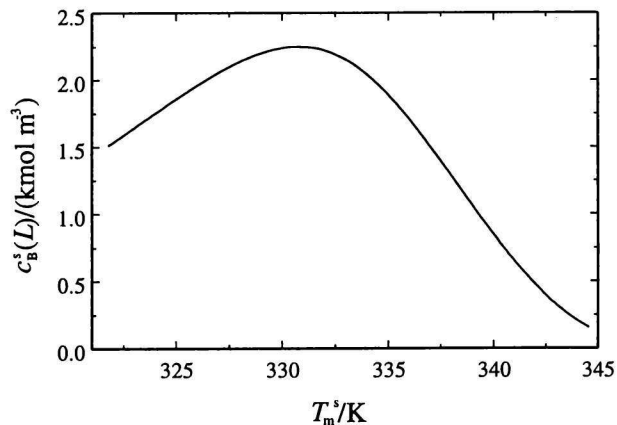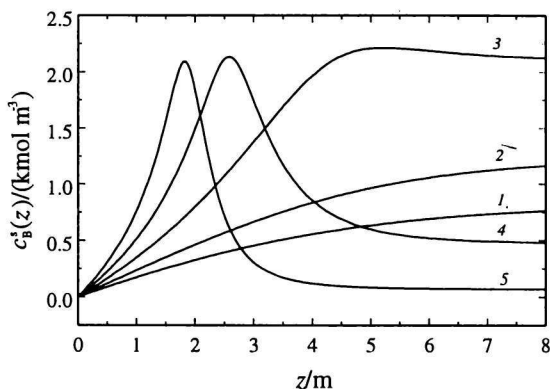

Fig. 3. Product concentration profiles for various inlet temperatures in a steady state. $T_{r0}^s/K = 219\ (1),\ 221\ (2),\ 223\ (3),\ 225\ (4),\ 227\ (5);\ q_c^s/(m^3\ s^{-1}) = 0.275$.
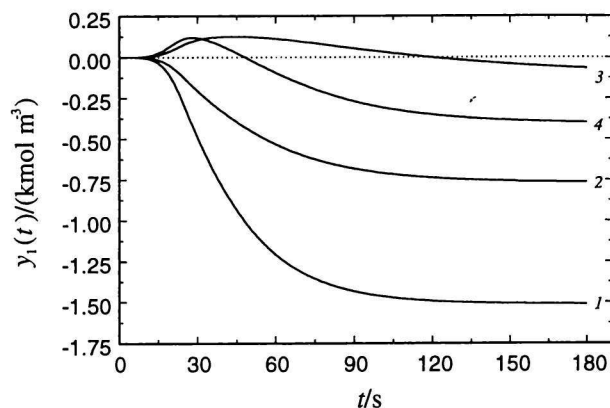

Fig. 4. Product outlet concentration *vs.* mean temperature in a steady state.

Fig. 5. The output y_1 time responses to input u step changes. $u/(m^3\ s^{-1}) = -0.05\ (1),\ -0.025\ (2),\ 0.025\ (3),\ 0.05\ (4)$.

Fig. 6. Time responses of outputs y_2 and y_3 to input u step changes. $u/(m^3\ s^{-1}) = -0.05\ (1),\ -0.025\ (2),\ 0.025\ (3),\ 0.05\ (4)$.

three outputs choices were considered and defined as deviations from their steady-state values, $u(t) = q_c(t) - q_c^s$, $y_1(t) = c_B(L,t) - c_B^s(L)$, $y_2(t) = T_r(L,t) - T_r^s(L)$, and $y_3(t) = T_m(t) - T_m^s$, where $q_c^s = 0.275\ m^3\ s^{-1}$.

The output y_1 time responses shown in Fig. 5 exhibit all negative properties from the control point of view. Non-minimum phase behaviour, varying sign of the gain as well as the significant time delay for this output are clearly documented. Both outputs y_2 and y_3 time responses in Fig. 6 show minimum phase properties and constant sign of the gain. However, the time delay of the output y_3 is less than the corresponding time delay of y_2.

CONCLUSION

The simulation results presented above clearly show that the mean temperature used as the controlled output has the best properties with respect to control purposes. Practically, the maximum of the re-
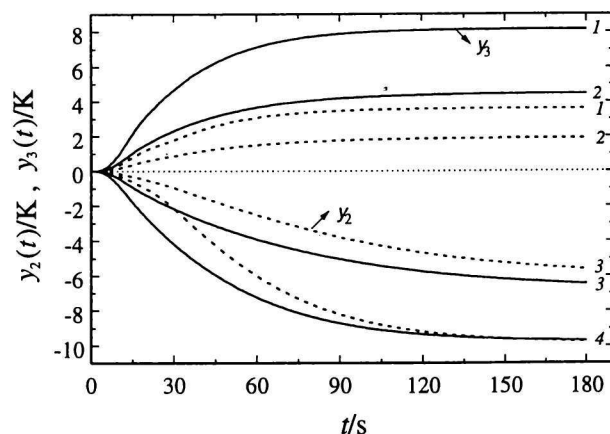
action product may be required as a control goal. The results of the steady-state analysis prove that the max-

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imum can be achieved through a suitable value of the mean temperature. In this case the mean temperature is controlled in the closed-loop by the given control variable (coolant flow rate). The desired (reference) value of the controlled variable is periodically computed and readjusted from the higher level of the control system depending on a measured product concentration. The control procedure is based on the principle called "Supervisory Control Strategy" . Moreover, the dynamic analysis results enable to determine the structure of the external linear model useful in many control strategies.

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